

## **Simulation of radiation environment in accelerators and accelerator driven systems**

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**Abstract** Estimation of radiation levels around particle accelerators is assuming crucial importance for design of high energy accelerators and accelerator driven systems. Such estimations have to depend greatly on theoretical calculations as experimental data in this area is scantily available. This paper briefly discusses the development and current status of nuclear reaction model codes employed for the purpose of simulating radiation environment in accelerators and accelerator driven systems. The present situation regarding available nuclear data as well as computational models in this field is far from satisfactory.

**Keywords** Accelerators, radiation environment

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### **1. Introduction**

A knowledge of the radiation environment in accelerators and other nuclear installations is an indispensable part of radiation safety and is considered essential for sound development of nuclear technology. Estimation of neutron production from charged particle interactions and subsequent transport and interaction of these neutrons in the surrounding medium comprise the major task in simulating radiation environment around accelerators and accelerator driven systems. The need for theoretical calculations arise from the fact that it is almost impossible to measure experimentally the energy distributions of emitted radiations and the various radionuclides formed from an overwhelmingly large number of possible nuclear interactions. Moreover, experience in this field shows that direct use of experimental data is inconvenient and may often lead to ambiguous results due to the inconsistency of the data obtained in various measurements or different approaches to interpolation or extrapolation procedures. The computational techniques differ greatly depending on the energy of the accelerated particles (*viz.* low, medium and high). At low energies evaporation process from the target-projectile composite system is of importance whereas at medium energies additional pre-equilibrium and direct reactions play important roles. At high energies development of nuclear cascades takes place initiated by energetic hadrons giving rise to a large number of particles principally nucleons, pions and kaons. Deep in the surrounding medium neutron takes on the dominant

role in cascade propagation below about 450 MeV where the ionization energy loss is significant for charged particles and pions.

Protons or other projectiles of 1 GeV and up, interacting with high Z-targets emit a large number of neutrons, leading to interesting possibilities of an accelerator driven subcritical system for generation of power as well as for incineration of long lived actinides and other nuclear wastes [1]. In such accelerator driven systems, the cascade has two qualitatively different and successive physical regions : (i) a spallation driven, high energy phase ; and (ii) a neutron driven, fission dominated phase. Neutrons from the first phase act as a source for the second where the main physical process is the diffusion of neutrons which gradually lose energy by collision and increase in number by fissions and  $(n, 2n)$  reactions.

Because of their relatively high penetrating power and for the reasons outlined above, it is evident that neutrons play a crucial role in determining the radiation environment around an accelerator and thus estimation of neutron yield from various nuclear interactions becomes essential. In the following we discuss a few nuclear reaction models and computational techniques involved in the field of radiation physics with accelerators and accelerator driven systems.

## 2. Possible nuclear reactions

When an energetic projectile (nucleon or nucleus) approaches a nucleus (target) and interacts with its constituent nucleons, nuclear reactions take place resulting in emission of nucleons and clusters. Low and medium energy projectiles initiate nuclear reactions that can be categorized in three parts :

(i) single step direct (DIR) reactions to collective discrete states, analysed with the optical model and the Distorted Wave Born Approximation (DWBA) or coupled channel models. Giant resonances also belong to same class ; (ii) compound nuclear or equilibrium reactions (EQ) to the continuum, analysed with the classical Weisskopf-Ewing or the quantum mechanical Hauser-Feshbach model ; (iii) pre-equilibrium reactions (PEQ) analysed with semiclassical exciton, hybrid, Boltzmann master equation approach and quantum molecular dynamics models or quantum mechanical multistep direct, multistep compound models. The pre-equilibrium reaction mechanism constitutes the bridge between fast ( $\sim 10^{-23}$ s) direct processes and the slow ( $\sim 10^{-20}$  s) compound processes and provides an explanation for the observed high energy tails in ejectile energy distributions and the smoothly forward peaked angular distributions.

Since a large momentum transfer is involved, DIR emissions are strongly forward peaked, carry high energy and as a result populate the low lying states of the residual nucleus. The transition matrix operates for transitions between well defined initial and final states. A solution is obtained only when the quantum numbers of the final state to which the transition is taking place are well defined. But, for instance, there might be transitions taking place through a single step interaction to some low energy continuum in which case the theory is not applicable since one cannot then define the quantum numbers of the final state uniquely.

In compound nuclear emissions, the ejectiles are emitted from a statistically equilibrated compound nucleus formed by sharing the incoming energy among all the nucleons through a series of two-body interactions. The memory of the formation channel, including the incident particle motion is lost and as a consequence the emissions are governed only by the general conservation laws of energy, angular momentum and parity. The last two are responsible for

the ejectile angular distribution being symmetric about  $90^\circ$  centre-of-mass (C.M.) angle. The incoming energy being shared amongst all the nucleons, the excitation energy per particle is small resulting in low energy emissions. The equilibrium statistical model [2, 3] explaining the experimental observations in support of compound nuclear reactions have been in use over several decades. The theory could explain the low energy emissions together with the observed angular distributions. But with increasing energy the equilibrium assumption becomes progressively poorer and the relaxation process prior to the equilibration needs to be followed. Indeed nuclear reactions at excitations of several tens of MeVs are complicated phenomena involving nucleon, cluster and collective excitations.

The PEQ emissions which occur during the relaxation process lie in between the DIR and EQ processes in ejectile energies since for the PEQ process excitation energy per particle is larger compared to what is observed when equilibrium is reached. The particles are emitted as the composite system proceeds towards a statistical equilibrium. The memory of the incident channel is still retained to some extent and the emissions are forward peaked with significant contributions at back angles. The DIR and EQ emissions have been studied in detail over a long period and there exist a number of well established theories explaining them. On the other hand, PEQ reactions are yet to be understood as fully as them. There are several models explaining the precompound reactions but most of them are incomplete in the sense that, though they account for the total cross section and energy distribution well, the angular distribution of the PEQ ejectiles are not fully explained.

For incident energies above *e.g.* 800 MeV, single and at higher energies multiple pion production becomes significant. At about 1 GeV, 20% to 30% of the primary-energy is radiated as pions but the production fall off steeply with increasing energy. The muons exhibit an increasing production rate with increase in energy and current in accelerators above 30 GeV. Charged pions and kaons decay into muons. Muons have no strong interactions and are stopped only by ionization energy losses. Energetic gamma rays produced in the decay of neutral pions initiate electromagnetic cascades but with shorter attenuation lengths. High energy electrons produce energetic hadrons, principally by photo disintegration of pseudo deuterons within the nucleus or by photo production of energetic pions, which are then reabsorbed within the nucleus. The resultant high energy neutrons and protons also can then generate nuclear cascade.

### 3. Nuclear reaction model codes

In the early years of 1960, simple models of nuclear cascade were used which could not reveal more than qualitative features of nuclear cascade development. More sophisticated analytical models yielded approximate solutions to the Boltzmann transport equations describing the cascade growth. Based on the experience at the Berkeley accelerators, Moyer [4] developed a phenomenological model capable of estimating the additional shielding required as a part of the Bevatron programme. The model worked fairly well for the specific purpose for which it was developed and was later on generalized to some extent. But several simplifying assumptions go into the model and as such the model cannot be considered rigorous.

Since that time substantial efforts have been directed toward application of Monte Carlo techniques to the calculation of nuclear cascade development. Under this scheme theoretical calculations of the intranuclear cascade, such as those due to Bertini [5] provided

increasingly reliable input information for the Monte Carlo routines. It is learned from the brief history of the subject that, of the variety of deterministic methods which looked promising in the 1960's with their mathematical elegance and efficiency of numerical techniques, none did determine the ultimate course of development to the stage of a practical design tool. For such reasons, Monte Carlo intranuclear cascade programs are used more and more in determining accelerator radiation environment. Among the various codes available for such purposes, the codes FLUKA [6], developed in the CERN and LCS [7] developed in the Los Alamos National Laboratory stand out. Both the codes are based on intranuclear cascade models.

FLUKA, originally a simple hadronic code, has been extended recently to deal with the transport of electrons, photons, low energy neutrons and muons. FLUKA is an integrated code which can treat in the same run complete hadronic cascade (generation and transport of about 30 different particles) over an energy range spanning more than 14 orders of magnitude. Several options of variance reducing schemes are available in the code. Hadron interactions in FLUKA are simulated using different models, depending on the energy of the primary particles. A Dual Parton Model is used above 5 GeV/c while a model based on resonance production and decay is used at lower energies. A cascade plus pre-equilibrium model is used below 300 MeV and a nuclear evaporation model is incorporated, accounting for the emission of neutrons, protons, heavy fragments and gamma rays from excited nuclei. FLUKA considers the photo nuclear reactions to proceed via the Giant Dipole Resonance below about 30 MeV, between 30 MeV and 200 MeV the Levinger quasi deuteron absorption mechanism, [8]. Above 140 MeV, the energy threshold for pion production, photonuclear interactions are characterized by excitation of the delta-resonance. In the high energy above the delta resonance, the Vector Meson Dominance Model [9] is used.

The LCS (Lahet Code System), based on coupling LAHET (LANL version of the HETC [10]) Monte Carlo Code) to MCNP (Monte Carlo Neutral Particle transport), is a system of code for calculating the transport of nucleons, pions and muons together with the continuous energy coupled neutron-photon transport. LCS includes as user option two models for fission induced by high energy interactions : the ORNL model by Alsmiller and others, and the Rutherford Appleton Laboratory model by Atchinson ; the fission models are employed with the evaporation model of Bertini to describe the physics of nuclear interactions. In LAHET, an alternative intranuclear cascade model has been adapted from the ISABEL Code which allows hydrogen and helium ions and antiprotons as projectiles. The Fermi breakup model has replaced the evaporation model for the breakup of light nuclei. An optional multistage pre-equilibrium exciton model has been implemented as an intermediate stage between the intranuclear cascade and the evaporation phase of a nuclear interaction. Alternative level density parameterizations have been added. The code LAHET treats all interactions by protons, pions and muons, but treats neutron interactions only above a cut off energy of 20 MeV. Any neutron appearing below the cut off energy has its kinematic parameters recorded on a neutron file for subsequent transport by a Monte Carlo Code utilizing ENDF/B-based neutron cross-section libraries.

There are certain points worthy of attention in intranuclear cascade (INC) models. One of these is that INC results do not conserve energy, sometimes resulting in particle emissions beyond thermodynamic end points. This may be because of using fixed neutron proton binding energies which do not reproduce experimental Q-values. Another problem is the difficulty in calculating ejectile energy distributions at extreme forward angles. This includes problems in overestimating quasi-elastic scattering peak and generally not reproducing the inelastic spectra

very well. Historically, INC codes under predicted spectra at back angles. While some of the codes have improved on this, others still have the same problem.

Another model, employed in the intermediate and higher energy region by Harp, Miller and Bern [11], is the Boltzmann Master Equation (BME) model which considers the equilibration process to proceed through twobody interactions. The transition rates are computed from free nucleon-nucleon scattering cross sections. The energy range accessible to the particles is divided into computationally convenient energy bins and then the variation in occupation probability of the energy bins is followed with time. Thus both particle and hole numbers as well as their energy distributions are obtained as functions of time. Angular information is ignored and the approach is more analytic compared to the intra-nuclear cascade model.

The most widely used models for PEQ phenomenon are the exciton model, introduced by Griffin [12], and developed later by Braga-Marcazzan *et al* [13] and Kalbach [14] and the hybrid model of Blann [15]. In the exciton model each stage of the equilibration process is described by the number of degrees of freedom *i.e.* the number of excited particles and holes or the excitons. The reaction is assumed to proceed through two-body interactions. An equal probability distribution is assumed for all energies of the excited particles. The intermediate state density which is applied to determine the energy states available to the particles is the most important factor in this approach. There are two versions of the exciton model. The first determines the time evolution of the occupancy in each exciton state during the energy sharing process and is called the "master equation exciton model". The second one employs the exciton model in a much simpler closed form. It assumes that each two-body interaction always results in the creation of a particle-hole pair, thereby neglecting annihilation of a particle-hole pair or redistribution of energy between the same number of excitons. This is known as "never-come-back" approximation. For high energy emissions this approximation is fairly good, but becomes questionable for determining angular distributions or low energy emission cross sections.

While following the relaxation process the hybrid model combines the BME and the exciton models. The relaxation process is characterized in terms of the exciton number as in the closed form of the exciton model. However, instead of assuming the occurrence of all energy distributions with equal probabilities, the hybrid model explicitly evaluates the pre-emission energy distribution of the ejectile in terms of appropriate state densities at each stage of the relaxation process. A more elaborate version of the hybrid model is the geometry dependent hybrid (GDH) model that includes nuclear surface effects. The effect of reduced matter density on the two body interaction rates as well as the effect of shallower potential depth on the permissible maximum hole energy at the nuclear surface are considered.

All the models mentioned above to explain pre-equilibrium reactions are semi-classical in nature. In a quantum mechanical approach, Feshbach, Kerman and Koonin (FKK theory) [16] suggested that the PEQ emissions take place either through a multi-step direct (MSD) or through a multi-step compound (MSC) mechanism. The former is responsible for the forward peaked angular distributions and the latter gives an angular distribution symmetric about 90° C.M. angle as in EQ emissions but with relatively higher emission energies. One advantage of this theory is its predictability of the PEQ angular distributions. However, the theory has so far been applied to nucleon emissions in light ion induced reactions only and could not, so far, be used for heavy ion projectiles. In a recent work [17] the FKK formalism has been used to study ( $p, \alpha$ ) reactions but as DIR emission rather than as PEQ.

Unlike the FKK formalism the exciton and the hybrid models deal with the energy spectra only and ejectile angular distribution cannot be described. The first calculations for PEQ angular distributions were performed using the intra-nuclear cascade model but it completely failed to account for the back angle emissions. Modifications were introduced in the exciton and the hybrid model so as to extend them to angular distribution calculations [18]. Mantzourains *et al* [19] described the PEQ angular distribution from master equation approach of the exciton model and included an angle dependent part in the transition rates. Most of these approaches are only partially successful, explaining the forward angle emissions quite satisfactorily. The back angle emissions are underpredicted, sometimes as much as by an order of magnitude. The Kalbach-Mann [18] systematics predicts the angular distribution fairly well but are based on empirical parameterization. Angular distribution in pre-equilibrium reactions are also calculated from the multiple nucleon-nucleon scattering kinematics inside the nuclear matter. The problem, however, lies in describing the motion of the target nucleons. Earlier, for nucleon induced reactions, the momenta of the nucleons were described by a zero-temperature Fermi distribution throughout the relaxation process and the two-body scattering kinematics evaluated therefrom resulting in severe underprediction of back-angle cross sections. In later approaches [20, 21], the excitation of the composite nucleus was taken into account and the nucleon momenta was described by a finite temperature Fermi distribution where the temperature was uniquely defined by the excitation. The resulting scattering kinematics gives good agreement with observed angular distributions.

The phenomena of heavy ion reactions are far more complicated than that of nucleon or light ion reactions. Deep inelastic scattering, quasi-elastic transfer reactions, fast fission processes, Fermi jet emissions contribute significantly to the total reaction cross section together with PEQ and EQ emissions. So far as PEQ emissions are concerned, the BME model has been used more or less successfully to analyze the energy spectra of nucleons and clusters [22], but with no angular information.

The theory of quantum molecular dynamics (QMD) [23, 24], originally formulated for heavy ion reactions and later extended for nucleon induced reactions is a semi-classical simulation method in which the nucleons are represented by gaussian wave packets. The distribution function for the total system is the sum of all nucleon wave packets. The time evolution of every nucleon is traced in event by event simulations (Monte Carlo) through Newtonian equations of motion in the self consistent mean field and stochastic two body collision processes. The time dependent variational principle is applied to the Newtonian equations using a Hamiltonian that consists of kinetic part, Skryme and Coulomb interaction part and the symmetry energy. The two nucleon collision which takes into account the Pauli blocking in the final state is also introduced. The change in the relative importance of the mean field effects and the two body collisions describe a transition between equilibrium, pre-equilibrium and spallation mechanisms including fast multi-particle emissions. The QMD theory is combined with a statistical decay model (SDM) to estimate evaporation from residual nuclei following fast particle emissions. The model predicts the angular distribution for nucleons as well as clusters.

Most of these PEQ models suffer from a lack of proper theory of multiple pre-equilibrium emission where more than one fast particle is emitted. It is quite established that above about

50 MeV incident energy such processes should be included when inclusive proton and neutron spectra are analysed. The QMD theory, however, automatically includes fast multiparticle emission processes since the time evolution of the degrees of freedom of every nucleon is considered explicitly. Deterministic PEQ calculations below 200 MeV (both semiclassical and quantum) have usually made the simplifying assumption that it is only sufficient to include a maximum of two fast particle emissions before a statistical evaporation model is used. Another drawback of the PEQ models is the absence of proper cluster emission calculations. It is felt that there may not be a good theory for predicting yields of clusters, beyond those which evaporate at equilibrium except some very recent efforts to develop models to predict non-equilibrium cluster emission. The QMD, however, considers cluster emission though it leaves scope for assessing its predictive capability.

It is this calculation of nucleon energy angle distribution emitted from nuclear reactions that links accelerators and accelerator driven systems while simulating their radiation environment. Production and analysis of double differential spectra and multiplicities obtained in the proton induced spallation reactions on various targets are of considerable interest of the ADS.

Central to the concept of the ADS is a medium energy (around 1 GeV) high current proton accelerator producing a beam of protons which stops on a heavy target resulting in a copious number of neutrons. These neutrons then drive a subcritical blanket assembly whereby they multiply in intensity and total energy thereby leading to an amplification of energy supplied in the form of the proton beam. These intense source of neutrons can then be used in several ways namely, energy production, transmutation of long lived wastes, burning of excess plutonium. The last two are by products of nuclear reactors mostly used for electricity generation.

Design and feasibility studies of ADS obviously require detailed transport calculations of radiations associated with stopping of protons of about 1 GeV in various target materials. Such calculations require information of nuclear interaction by protons and neutrons from essentially very low energies up to the primary beam energy with target and structural materials, coolants, fissile blanket materials, fission and spallation products and actinides.

For a detailed study of such accelerator driven system, the LCS is a code that can be used directly, since LCS can successfully simulate both the high and low energy phases required for the present calculation. After the production of spallation neutrons the phenomenology is similar to that of nuclear reactors. However, because the system is not critical, there are important differences : in a reactor the flux distribution inside the volume is determined essentially by the boundaries, in the ADSS the location and geometry of the initial cascade acting as neutron source is dominant. The neutron source excites a superposition of orthonormal modes of the buckling equation representing the neutron flux, of which only the fundamental mode is relevant to a reactor theory. In this description, a reactor is a limiting case in which the strength of the initiating source tends to zero and the criticality to one. Each of these modes has a different buckling parameter and a different multiplication coefficient. As a consequence, (i) the spatial neutron flux is expected to decay exponentially from the point of the source, rather than having the characteristic cosine distribution centred with respect to the volume as in a critical reactor ; and (ii) for a proton pulse sharp in time (delta-function), the neutron population decreases exponentially with a time constant which grows linearly with  $1/(1 - k_{eff})$ , where  $k_{eff}$  is the effective multiplication coefficient.